(E)-3-Phenyl-1-(piperidin-1-yl)prop-2-en-1-one

Inchi: InChI=1S/C14H17NO/c16-14(15-11-5-2-6-12-15)10-9-13-7-3-1-4-8-13/h1,3-4,7-10H,2,5-
InchiKey: KNOXUMZPTHELAO-MDZDMXLPSA-N
Formula: C14H17NO
SMILES: O=C(C=Cc1ccccc1)N1CCCCC1
Mol. weight [g/mol]: 215.29
CAS: 27845-72-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	2.712		Crippen Method
mcvol	180.750	ml/mol	McGowan Method
rinpol	2118.40		NIST Webbook
rinpol	2118.40		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27845723&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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